APPENDIX A:

**ENVIRONMENTAL FATE AND TOXICITY OF ACWA VESICANTS,
NERVE AGENTS, AND THEIR DEGRADATION PRODUCTS**

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A.1 INTRODUCTION

This appendix discusses the fate and toxicity of ACWA chemical warfare agents (CWAs) and their degradation products. Two broad classes of CWAs are considered: vesicants (blister agents; i.e., compounds that cause blisters, such as mustard) and nerve agents (compounds that affect the nervous system). The vesicants discussed are HD, HT, and H; the nerve agents discussed are VX and GB. Data on the principal degradation products of the vesicants and nerve agents are also provided. The information presented is useful for impact analyses and covers both physical and chemical properties.

The fate of CWAs and their degradation products in the environment is discussed in terms of the following four processes: photolysis, hydrolysis, oxidation, and microbial degradation. Photolysis is the chemical decomposition of a CWA by sunlight. This process is relevant for surface spills. Hydrolysis is the decomposition of a CWA by its chemical reaction with water. Hydrolysis is pertinent to CWAs buried in moist soil, inadvertent releases or spills into surface water bodies, and surface spills that are exposed to precipitation (Munro et al. 1999). Oxidation is the decomposition of CWA by chemical interaction with oxygen. Oxidation also occurs when an agent's valence state (ionic charge) is increased positively (e.g., +1 to +2) or decreased negatively (e.g., –2 to –1) as a result of this interaction. Oxidation is relevant to chemical warfare (CW) compounds in contact with air or natural oxidants in the soil or water. Microbial degradation is decomposition of CWA by interaction with living microbes. This process is of interest when CW material is either on soil or buried in it and active communities of CWA-degrading microbes are present. CWAs that have low rates of photolysis, hydrolysis, oxidation, or microbial degradation are classified as persistent in the environment.

Even though a CWA may be persistent in the environment, its presence may not be significant if its toxicity (ability to harm humans, other animals, fish, and plants) is low. Toxicity depends on the exposure pathway (Munro et al. 1999). These pathways include oral (introduced through the mouth), inhalation (introduced by breathing), and dermal (introduced by skin contact). Lethal compounds that produce death to 50% of tested animals (lethal dose of 50%, or LD_{50}) or that produce death at a median concentration (lethal concentration of 50%, LC_{50}) at levels of less than 50 mg/kg (oral), less than 50 mg/m^3 (inhalation), and less than 200 mg/kg (dermal) after a single exposure are highly acutely toxic. Compounds with LD_{50} or LC_{50} values of 50–500 mg/kg (oral), 50–500 mg/m^3 (inhalation), or 200–500 mg/kg (dermal) are moderately toxic. Compounds with even higher values for LD_{50} and LC_{50} have a low toxicity. Toxic chronic (long-term) exposures are generally an order of magnitude lower than the above numbers. For aquatic organisms, LC_{50} values of less than 1 mg/L are highly acutely toxic, and LC_{50} values of less than 0.1 mg/L are chronically toxic.

The remainder of this appendix discusses the fate and toxicity of mustard (HD, HT, and H), the nerve agents VX and GB, and their major degradation products.

A.2 VESICANTS

Vesicants (blister agents) are CW compounds that produce blistering over the entire body, including the eyes and lungs. Although lethal, vesicants are designed to maim rather than kill. In World War I, mustard was a very effective incapacitating agent, despite producing only 1% fatalities among its casualties (Mitretek 2000a). Three vesicants are discussed in this appendix: HD, HT, and H. In the pure form, all are colorless and odorless. Agent-grade material is typically pale yellow to dark brown with a smell similar to burning garlic (Mitretek 2000b).

Chemical weapons disperse mustard as an aerosol, which then evaporates to produce contaminated vapor. After exposure to the vapor, delayed tissue damage occurs within minutes of contact. Clinical effects are not immediately evident; they are manifested 2 to 24 hours after exposure (Stimson Center 2000). Topical effects occur on the skin (blisters), in airways (coughing, lesions, and, in rare cases, respiratory failure), and in the eyes (itchiness, a burning sensation, and possible damage to the cornea). Nausea and vomiting can also result.

Most of the stored mustard for the ACWA program is in the distilled or purified form of sulfur mustard (HD). HT was made by an older manufacturing process and contains about 60% HD, less than 40% of the agent T (bis[2-(2-chloroethylthio)ethyl]ether), and a variety of sulfur contaminants and impurities (Munro et al. 1999). HT may have many of the same toxic effects as HD; however, very few studies on HT are available in the literature. H is an undistilled mustard that also contains impurities. H has the chemical name 1,1'-thiobis[2-chloroethane]. Its molecular formula is $C_4H_8Cl_2S$, and its formula weight is 159.08 g/mole. Its properties have not been reported in the literature; however, its toxic properties are believed to be similar to those of HD. A 1-ton container of HD manufactured after World War II contains approximately 89% HD. Older processes used prior to World War II (such as the Levinstein process) produced mustards that contained 62 to 64% HD. Chemical and physical properties of HD, HT, and H are given in Table A.1.

Sulfur mustard is considered to be fairly persistent in the environment (Munro et al 1999). At moderate temperatures (25°C), HD deposited on the surface of soil will evaporate within 30 to 50 hours, depending on weather conditions. Predicted persistence times for drops applied to soils at a rate of 50 g/m^2 for various conditions of wind and rain were 1,122 to 2,215 hours at 0°C and 30.5 to 51.2 hours at 25°C (Munro et al. 1999). At lower temperatures (less than 13 to 15°C, mustard freezes (Table A.1). Studies of the persistence of mustard performed at low temperatures (–1°C) in Norway show that small, solid particles formed on the surface of any snow that was present. The droplets disappeared fairly rapidly, primarily through evaporation. After two weeks, only 0.0001% remained (Munro et al. 1999). This rate of removal corresponds to an effective half-life (the amount of time needed for one-half of the mustard to decompose) of about 0.7 day.

TABLE A.1 Physical and Chemical Properties of CWAs

Property	HD/H	HT	VX	GB
Molecular weight	159.08	Nd[a]	267.4	140.1
Physical state	Oily liquid	Oily liquid	Oily liquid	Liquid
Color	Clear/pale yellow, black if impure	Amber/dark brown	Light amber/ amber	Colorless
Melting point (°C)	13–14	1	–39 (calculated)	–56
Boiling point (°C)	215–217	>228	298 (decomposes)	158
Density (g/mL)	1.27 at 20°C	1.27 at 20°C	1.008 at 20°C	1.102 at 20°C
Vapor pressure (mmHg at 20 or 25°C)	0.11	0.10	0.0007	2.10
Volatility (mg/m^3)	920	831	10.5	22,000
Solubility in water (g/L)	0.92	Almost Insoluble	30	Miscible
Hydrolysis half-life	8.5 min	ND	1,000 h (pH = 7)	39 h (pH = 7)
Henry's Law constant (atm $\times$ m^3/mol)	2.1×10^{-5}	ND	3.5×10^{-9}	5.4×10^{-7}
Log K_{ow}	1.37	ND	2.09	0.299
Log K_{oc}	2.12	ND	2.5	1.77

[a] ND = No data found.

Source: Munro et al. (1999).

Because mustard does not absorb ultraviolet radiation, photodegradation does not appear to be a significant degradation process (Munro et al. 1999). However, HD will decompose in the air by reaction with hydroxyl (OH$^-$) radicals. In the presence of hydroxyl radicals produced by sunlight in air containing water vapor, HD has an apparent half-life of about 1.4 days.

U.S. Army Center for Health Promotion and Preventive Medicine (2002) reported that HD spilled into seawater would probably sink because it is more dense than water. (HD has a specific gravity [ratio of compound density to the density of water] of 1.27 at 20°C.) Once in water, the mustard would dissolve. Compounds are considered to be moderately to highly soluble if their solubility is greater than 1 g/L. Because the solubility of mustard is about 0.8 g/L at 20°C

(Table A.1), the dissolution process would be slow (Munro et al. 1999). The dissolved mustard would mix with the surrounding water and undergo hydrolysis, which would quickly reduce its concentration.

If the mustard was buried in an unsaturated soil (i.e., one in which the pore spaces are not completely filled with water), the mustard could decompose by a combination of dissolution and vaporization. As mentioned above, dissolution would be slow. Vaporization, on the other hand, could occur at a moderate pace because its Henry's Law constant (ratio of the concentration in the vapor phase to the concentration in the liquid phase) is 2.4×10^{-5} atm $\times$ m^3/mol (Munro et al. 1999). Dissolution could reduce the rate of volatilization by causing intermediate hydrolysis products to form that would coat the surface of the mustard drop. The volatilization rate is further decreased at low temperatures (e.g., mustard freezes at temperatures less than 13 to 15°C). Under conditions of low relative humidity (27 to 35%) and temperatures ranging from 21 to 25.5°C, 7 to 32% of mustard experimentally applied to soils was recovered in the first 6 hours. By the time volatilization ended (15 to 55 hours), 12 to 66% had been recovered. The rate of mustard vapor generation and recovery depended on the soil pH, moisture content of the soil, and the chemical and physical properties of the soil (Munro et al. 1999).

The principal environmental degradation process for stored or buried HD is hydrolysis. Hydrolysis is controlled by surface reactions, with products formed at the HD-water interface and then diffused into the bulk-water phase. Once in the water phase, HD has an estimated hydrolysis half-life of 4 to 8 minutes (Munro et al. 1999). However, its rate is limited by the slow rate of dissolution. Mustard has been known to persist for decades under water (Mitretek 2000b). The rate of dissolution can be further reduced by the formation of intermediate hydrolysis products that coat the mustard droplets.

Mustard can be theoretically biodegraded in soil via the thioether oxidation pathway to form bis(2-chloroethyl)sulfoxide and a corresponding sulfone, both of which are soluble in water (Munro et al. 1999). Mustard can also be biodegraded by reductive dehalogenation and dehydrohalogenation; however, these pathways are predicted to be very slow. Although biodegradation of mustard has been predicted, it has not been demonstrated successfully in the laboratory, probably because of its toxicity to microorganisms.

Many organic compounds that are dissolved in water can be adsorbed onto solid surfaces through a process termed the hydrophobic effect (Fetter 1993). The partitioning of a solute onto mineral surfaces or organic carbon in a soil primarily depends on the fraction of organic material, f_{oc}, present. Under these conditions, a partition coefficient with respect to the organic fraction K_{oc} is defined as:

$$K_d = f_{oc} \, K_{oc} \,, \tag{1}$$

where K_d is the mass of solute on the solid phase per unit mass of solid phase divided by the concentration of solute in solution. As indicated in Table A.1, K_{oc} for HD is approximately 132. If

organic matter is present in the soil at typical values (1 to 3%), the partition coefficient for HD would range from about 1 to 4 mL/g. If the partition coefficient were 0.0 mL/g, there would be no retardation of the mustard with respect to the velocity of the groundwater (i.e., the mustard would travel at the same velocity as the groundwater).

The amount of retardation, R, can be calculated by using the following relationship from Freeze and Cherry (1979):

$$R = 1 + (P_b K_d / \varphi),\tag{2}$$

where ρ_b is the bulk density of the soil and φ is its effective porosity (ratio of the volume of interconnected voids to the volume of the soil). For a bulk density of 1.7 g/cm^3 and an effective porosity of 0.3, mustard would travel up to about 20 times slower than the water in which it is dissolved.

Table A.1 also provides information on another physical parameter important for analyzing the impacts of the presence of mustard in water: K_{ow}, the octanol-water partition coefficient (Fetter 1993). This parameter provides an estimate of a chemical's tendency to bioaccumulate in organisms. High values of K_{ow} (or log K_{ow}) indicate that a substance will tend to concentrate in soil organic matter or in fatty tissue in the body (Rosenblatt et al. 1995).

For various organic materials, there is a relationship between the octanol-water partition coefficient and K_{oc}. For many organics, this relationship is given by the following equation from Fetter (1993): $K_{oc} = 0.63 K_{ow}$.

$$K_{oc} = 0.63 K_{ow} .\tag{3}$$

The principal degradation products of mustard undergoing hydrolysis are thiodiglycol (TDG) and hydrochloric acid (Munro et al. 1999). The major hydrolysis products of HT and T after overnight hydrolysis at 50°C were TDG, hemisulfurmustard, 2-chloroethyl(2-hydroxyethylthio)-ethyl ether, bis(2-hydroxyethylthio)ethane, mustard agent, and 1,4-dithiane (Munro et al. 1999). Table A.2 presents a list of mustard degradation products and their physical properties. TDG is stable in the absence of water, is miscible with water, and has a half-life in aqueous solution of about 6 weeks. No aqueous photolysis occurred when aqueous solutions of TDG were exposed to sunlight for 14 days. TDG can be possibly oxidized to TDG sulfoxide and TDG sulfone. TDG, 2-chloroethyl vinyl sulfone, and divinyl sulfone are essentially nonvolatile (will not form vapors). Divinyl sulfide and 1,2-dichloroethane rapidly form a gas phase. Hemisulfur is not expected to persist in the environment, and it decomposes rapidly by hydrolysis.

Two common degradation products of HD that are persistent in the environment are 1,4-oxathiane and 1,4-dithiane (Table A.2). 1,4-oxathiane is formed by dehyrohalogenation of partially

TABLE A.2 Physical Properties of Mustard Degradation Products[a]

Compound	Water Solubility (g/L)	Log K_{ow}	Log K_{oc}	Vapor Pressure (mmHg)
Sulfur mustard	1.0	1.37	2.12	0.1
Thidiglycol (TDG)	Miscible	–0.77	0.96	0.00002
2-Chloroethyl vinyl sulfide	1.4	1.11	1.98	5.8
Divinyl sulfide	2.5	–0.85	1.84	6.0
Mustard sulfoxide	93	–0.85	0.91	0.65
Mustard sulfone	11	–0.51	1.11	0.96
2-Chlorovinyl sulfoxide	160	–1.11	0.77	0.064
Vinyl sulfoxide	280	–1.37	0.63	0.92
2-Hydroxyethyl vinyl sulfide	5.0	0.53	1.66	3.8
2-Chloroethyl vinyl sulfone	78	–0.77	0.96	0.023
Divinyl sulfone	140	–1.03	0.82	0.09
1,4-Dithiane	3.0	0.77	1.80	0.80
1,4-Oxathiane	167	0.60	ND	3.9
1,2-Dichloroethane	11	1.48	2.18	8.5

[a]K_{ow} = Octanol water partition coefficient, an estimate of a chemical's tendency to bioaccumulate in organisms. High values of K_{ow} indicate that a substance will tend to concentrate in soil organic matter or in fatty tissue rather than in water (Rosenblatt et al. 1995).

K_{oc} = Organic carbon partition coefficient, an estimate of the tendency of a chemical to absorb to the organic carbon phase in soil or sediment. The greater the value of K_{oc}, the greater the tendency of a substance to stick to organic matter in soil and not migrate with water or vaporize into the air (Rosenblatt et al. 1995).

Source: Munro et al. (1999)

hydrolyzed mustard, whereas 1,4-dithiane is a thermal degradation product of mustard formed by dechlorination. Both compounds are contaminants in the Rocky Mountain Arsenal area near Denver, Colorado (Munro et al. 1999), and 1,4-dithiane has been identified in groundwater at Aberdeen Proving Ground, Maryland. 1,4-Dithiane readily vaporizes from both soil and surface water. It also photooxidizes to form sulfoxides and sulfones.

In addition to hydrolysis, TDG is also susceptible to biodegradation (Munro et al.1999). When mustard was hydrolyzed prior to inoculation with *Pseudomonas pickettii* (SH18) and *Alcaligens xylosoxidans* (ssp. *Xylosoxidans* strain SH42), up to 97% of the carbon-containing hydrolysis products were degraded. TDG was completely degraded by *A. xylosoxidans* strain SH91 in a laboratory-scale stirred-tank reactor. No associated rates of degradation are available.

Mustard has strong alkylating properties and consequently demonstrates systemic toxicity (i.e., affects the entire organism) in addition to its effects on skin, eyes, and the respiratory tract (Munro et al. 1999). Mustard is also considered to be a known human carcinogen. Its LD_{50} is reported to be 4,500 mg/kg of body weight and its LC_{t50} is reported to be 1,500 mg/min/m^3 (Stimson Center 2000). TDG, the principal hydrolysis degradation product, exhibits low to very slight toxicity and does not retain the vesicant properties of the parent. Oral doses in the range of 4 to 6 g/kg were required to produce 50% lethality in rodents.

Hemisulfur mustard is an intermediate degradation product formed in the course of HD hydrolysis to TDG. It retains some acute toxicity (0.1 to 0.25 times as toxic as HD in mice for dermal and intravenous pathways) (Munro et al. 1999). Acute toxicity data for 1,4-dithiane suggest low lethality; the oral LD_{50} value for rats is about 3.5 g/kg body weight. The acute toxicity of 1,4-oxathiane is also relatively low, with LD_{50} oral values in rats of about 3 g/kg body weight. A more complete summary of toxicity information for vesicant degradation products is provided in Munro et al. (1999).

In summary, the CW vesicants HD, HT, and H can persist in the environment. Agents on the soil will evaporate and then hydrolyze. Agents in surface water will volatilize and decompose by hydrolysis. Agents under water will dissolve slowly and then quickly hydrolyze. Agents buried in the unsaturated zone will vaporize, dissolve slowly, and hydrolyze quickly. Agents in the zone of saturated groundwater will dissolve slowly and then hydrolyze rapidly. Because the dissolution process for mustards is slow, agent can remain in place for a relatively long time. However, once dissolution has occurred, decomposition by hydrolysis is rapid, and advective transport in moving water is slower than the groundwater velocity. After decomposition, mustard degradation products can persist in the environment, although some of these degradation products will vaporize and hydrolyze readily. Identification of these products can indicate the presence of potential mustard sources.

The lethality of mustard and its associated degradation products is low, as indicated by the LD_{50} values. This finding is consistent with the understanding that vesicants are not designed for lethality. Rather, they are designed to be effective incapacitating agents.

A.3 NERVE AGENTS

All CW nerve agents are strong inhibitors of enzymes found in the body. In particular, nerve agents inhibit the enzyme acetylcholinesterase, therby allowing acetylcholine to build up at nerve synapses. The accumulation of acetycholine at these sites effectively prevents the transmission of nerve signals in the body (Mitretek 2000c).

After exposure to a CW nerve agent, incapacitating effects occur within 1 to 10 minutes; lethal effects occur within 2 to 15 minutes. Effects in the eyes include contraction of the pupils (meiosis), pain, and dim or blurred vision. A runny nose may occur, and there is a tightness in the chest. Nausea and vomiting are also possible. When skeletal muscle is reached by the agent, twitching and convulsions result. Fluctuations also occur in the heart. Loss of consciousness and seizure activity can occur within one minute of exposure to high concentrations. Eventual paralysis and death follow (Stimson Center 2000). The fate and toxicity of VX, GB, and their degradation products are discussed below.

A.3.1 VX

The CW nerve agent VX was first introduced in 1954 (Mitretek 2000d). It has the chemical name methylphosphonothioic acid, S-[2-[bis(1-methylethyl)amino]ethyl]-O-ethyl ester. It is a persistent, odorless, amber-colored liquid that has the molecular formula $C_{11}H_{26}NO_2PS$. It has a formula weight of 267.37 g/mole (Mitretek 2000e). VX is usually formulated with 1 to 3% stabliziers (e.g., diisopropyl carbodiimide) to protect it against decomposition by trace quantities of water.

VX is not very volatile (10.5 mg/m^3 at 25°C) and does not evaporate readily. Its Henry Law constant of 3.5×10^{-9} atm $\times$ m^3/mol indicates that it is essentially nonvolatile in water (Munro et al. 1999). VX is moderately persistent on the bare ground and may remain in significant concentrations for a period of two to six days, depending on the temperature, organic content of the soil, and moisture. The degradation results from a combination of evaporation, hydrolysis, and biodegradation. The effective half-life of VX in soil is considered to be about 4.5 days on the basis of estimates that show that 90% of initially applied VX in soil would be lost in less than 15 days.

VX is moderately to highly soluble in water, with a solubility of 30 g/L at 25°C (Munro et al. 1999). It is fairly resistant to hydrolysis. The reported half-life in water ranges from 17 to 42 days at a temperature of 25°C and a pH of 7. The rate of hydrolysis is temperature dependent (Kingery and Allen 1995). At lower temperatures, the degradation rate of VX decreases by a factor of ten for every 10°C. The degradation rate is also a function of the system pH. For slightly acidic conditions, the hydrolysis half-life is 100 days.

At neutral and alkaline pH values, the principal degradation product of VX is EA2192 (S-(2-diisopropylaminoethyl)methyl phosphonothioate), which is environmentally stable and infinitely

soluble in water. Other VX hydrolysis degradation products include EMPA (ethyl methylphosphonic acid) and DESH (diisoproplyethyl mercaptoamine). The half-life of EMPA is 8 days (Munro et al. 1999), with degradation to MPA (methylphosphonic acid). MPA is stable in the environment because it is resistant to hydrolysis, photolysis, and thermal decomposition. It is also very soluble in water and has a low coefficient for sorption onto soil particles. Other physical properties of the degradation products of VX are given in Table A.3.

The LD_{50} via skin contact for VX is 10 mg/kg body weight (Stimson Center 2000). Via inhalation, the LCt_{50} is 50 mg/min/m^3. Little is known about the toxicity of most of the hydrolysis degradation products of VX, although EA2192 retains its anticholinesterase activities. In environmentally relevant situations, EA2192 is not absorbed through the skin and unlikely to be inhaled. Only the oral pathway remains a concern. Its intravenous toxicity is somewhat lower (0.24 to 0.825) than VX. Its oral lethality in rats (630 µg/kg) is about 0.1 to 0.2 that of liquid VX. A conservative proposed reference dose, RfD, calculated by the U.S. Environmental Protection Agency (EPA) for EA2192, is 0.0006 µg/kg per day, which is the RfD for the more potent parent, VX. Although information about other VX degradation products is limited, it appears that none of them display the high acute toxicity of EA2192. Most of this information indicates that the degradation products have low to moderate lethality. A more complete discussion on the lethality of VX degradation products can be found in Munro et al. (1999).

A.3.2 G Agents

There are three principal CW G agents: GA (Tabun), GB (Sarin), and GD (Soman). GA contains a cyanide group; GB and GD contain a fluoride substituent group. GB and GD are methylphosphonofluoridate esters (Munro et al. 1991). Unlike the V agents, the G agents are volatile and present a vapor hazard. GA (Tabun; ethyl dimethylphosphoramidocyanidate or $C_5H_{11}N_2O_2P$) was first prepared by Gerard Schrader in 1934. GB (Sarin; methylethyl methylphosphonofluoridate or $C_4H_{10}FO_2P$) was discovered a little later in 1938. GD (Soman; methylphosphonofluoridate or $C_7H_{16}FO_2P$) was developed in 1944. All of the agents are colorless, odorless liquids that readily volatilize.

All of the G agents have incapacitating effects that occur within 1 to 10 minutes. Lethal effects of GA occur within 10 to 15 minutes, lethal effects for GB occur within 2 to 15 minutes, and lethal effects for GD occur within 1 to 15 minutes (Munro et al. 1999). As does VX, G agents affect the eyes (meiosis, pain, and dim or blurred vision), nose (runny), and chest (tightness). Nausea and vomiting are also possible. When skeletal muscles are reached, twitching and convulsions can occur, followed by fluctuations in the heart rate. Loss of consciousness and seizures can occur within one minute of exposure to high concentrations. Eventual paralysis and death follow (Stimson Center 2000).

In the United States, GA was produced in much smaller quantities than GB and VX. Nonstockpile material in glass ampules (0.07 lb of total material) is stored in a drum at Tooele Army Depot. Stockpiled amounts include 1.41 tons of the agent in two 1-ton containers and 0.64 ton of the

TABLE A.3 Physical Properties of the Degradation Products of VX

Compound	Water Solubility (mg/L)	Log K_{ow}	Log K_{oc}	Vapor Pressure (mmHg)
Ethyl methylphosphonic acid (EMPA)	1.8×10^{-5}	–1.15	0.75	3.6×10^{-4}
S-(2-diisopropylaminoethyl) methylphosphonothioic acid	Infinitely soluble	0.96	1.90	ND
Bis(2-disopropylaminoethyl) sulfide	1.2	4.47	3.81	2.7×10^{-7}
Bis(2-diisopropylaminoethyl) disulfide	9.5	3.48	3.28	5.9×10^{-9}
Ethyl methylphosphonothioic acid	1,100	1.26	2.06	0.043
Diisopropylaminoethanol	1,500	1.08	1.96	1.8
Methylphosphonic acid (MPA)	$>1 \times 10^{6}$	–2.28	0.15	2×10^{-6}
Diethyl dimethylpyro-phosphonate	$>1 \times 10^{6}$	–2.12	0.23	ND

Source: Munro et al. (1999).

thickened agent in two 1-ton containers. GD was also produced in low quantities in the United Sates and is not relevant for the ACWA project. Because of the small quantities of GA and GD produced, and their lack of relevance to the ACWA project, they will not be discussed further in this appendix.

GB is the most volatile of all of the G agents. It has a vapor pressure of 2.10 mmHg and volatility of 22,000 mg/m^3 (Munro et al. 1999). Because it vaporizes so readily, GB is largely a vapor hazard rather than a contact hazard. Because GB is also completely miscible with water, it can pose a threat to water resources.

In the environment, GB is considered to be nonpersistent (Munro et al. 1999). It is volatile, soluble in water, and subject to acid and base hydrolysis. A calculated volatilization half-life for GB is 7.7 hours. The low calculated Henry's Law constant, 5.4×10^{-7} atm $\times$ m^3/mol indicates slow to practically no volatilization from water. At 20°C and a neutral pH, estimates of the hydrolysis half-life of GB range from 46 hours (pH of 7.5) to 461 hours (pH of 6.5). GB is more persistent at low

temperatures; an effective hydrolysis half-life of 8,300 hours is estimated for a temperature of 0°C and pH of 6.5. GB hydrolyzes to form isopropyl methylphosphonic acid (IMPA) and hydrofluoric acid. A second, slower process produces MPA.

In soil, GB undergoes hydrolysis, evaporation, and leaching. The phosphonic acid hydrolysis products are subject to biodegradation (Munro et al. 1999). Studies indicate that 90% of GB is lost in the first five days. This loss rate corresponds to an effective half-life of 1.5 days. The half-life for hydrolysis depends on the pH of the receiving water. Measurements of its half-life at a pH of 6.5 range from 193 to 312 hours (Kingery and Allen 1995). GB is more persistent at low temperatures. Newly fallen snow in Norway protected GB droplets from evaporation for periods of two to four weeks. The hydrolysis product IMPA was present up to four weeks later.

The hydrolysis product IMPA is extremely stable. Its predicted half-life is longer than 1,900 years (Munro et al. 1999). Hydrolysis of IMPA produces MPA and isopropyl alcohol. The low vapor pressure of IMPA (0.0034 mmHg at 25°C) limits the possibility of atmospheric contamination. A moderate to high solubility (48 g/L) and a low organic distribution coefficient (K_{oc} = 12) indicate a high potential for migration to groundwater. Because of its low K_{oc} (Table A.3), MPA is also very mobile in the environment and can be readily transported by advection. Additional information on other degradation products of GB are found in Munro et al. (1999).

The LD_{50} for GB is 1,700 mg/kg body weight (Stimson Center 2000). Its LCt_{50} is 100 mg/min/m^3. IMPA has low oral toxicity in rats and mice; it produced only mild skin irritation and no eye irritation in rabbits (Munro et al. 1999). The EPA calculated oral RfD for the hydrolysis degradation product, IMPA, is 0.1 mg/kg/day. The EPA derived an adult lifetime drinking water health advisory value of 0.7 mg/L (Munro et al. 1999). MPA is considered to be a human skin and eye irritant with low to moderate toxicity. A calculated RfD for MPA is 20 μg/kg/day (Munro et al. 1999).

A.3.3 Nerve Agent Summary

Of the nerve agents included in this appendix, VX is environmentally persistent, whereas GB is not. VX is not very volatile, does not evaporate, and is nonvolatile when in water. However, it is moderately to highly soluble in water. VX on the soil degrades by dissolution, followed by hydrolysis. VX in water or underwater dissolves and then hydrolyzes. VX buried in the unsaturated zone or in the saturated groundwater zone dissolves with infiltrating precipitation. Hydrolysis of VX produces the stable and soluble degradation products EA2192 and MPA. Because EA2192 retains its anticholinesterase properties, it can be a potential threat to surface water and groundwater resources. The major pathway of concern for EA2192 is ingestion, since it is not absorbed through the skin and is not likely to be inhaled. As is EA2192, the degradation product MPA is stable and very mobile in the environment. However, MPA is a degradation product of low to moderate toxicity that is primarily a human eye and skin irritant.

GB is a nonpersistent CWA. It volatilizes readily, is miscible with water, and hydrolyzes. GB on the soil degrades by evaporation, dissolution, and hydrolysis. GB in water or underwater vaporizes, dissolves, and hydrolyzes. GB buried in the unsaturated zone or in the saturated groundwater zone vaporizes, dissolves with infiltrating precipitation, and hydrolyzes. The degradation products of GB include IMPA and MPA. IMPA is extremely stable in the environment, with a degradation half-life of about 1,900 years. In addition, it is transported readily by advecting groundwater. However, IMPA, like MPA, is not a major concern with regard to water contamination because of its low toxicity.

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